



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BPX  
Title : DNA POLYMERASE BETA/DNA COMPLEX  
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Deposited on : 1997-04-11  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

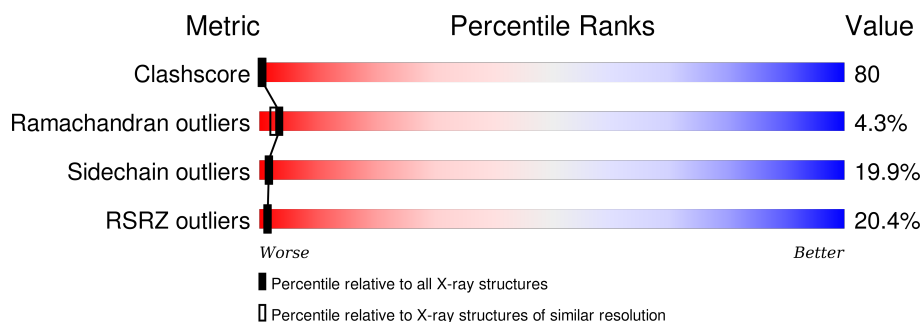
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	16	<div> <div>6%</div> <div>38%</div> <div>63%</div> </div>
2	P	10	<div> <div>10%</div> <div>10%</div> <div>90%</div> </div>
3	D	5	<div> <div>100%</div> </div>
4	A	335	<div> <div>21%</div> <div>19%</div> <div>50%</div> <div>24%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3368 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	16	Total	C	N	O	P	0	0	0
			323	153	63	92	15			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*TP\*CP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 4 is a protein called PROTEIN (DNA POLYMERASE BETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	331	Total	C	N	O	S	0	0	0
			2653	1676	464	504	9			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

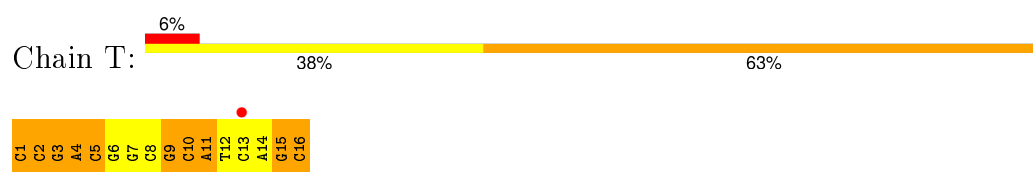
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	40	Total 40	O 40	0	0
6	D	6	Total 6	O 6	0	0
6	P	14	Total 14	O 14	0	0
6	T	21	Total 21	O 21	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3')



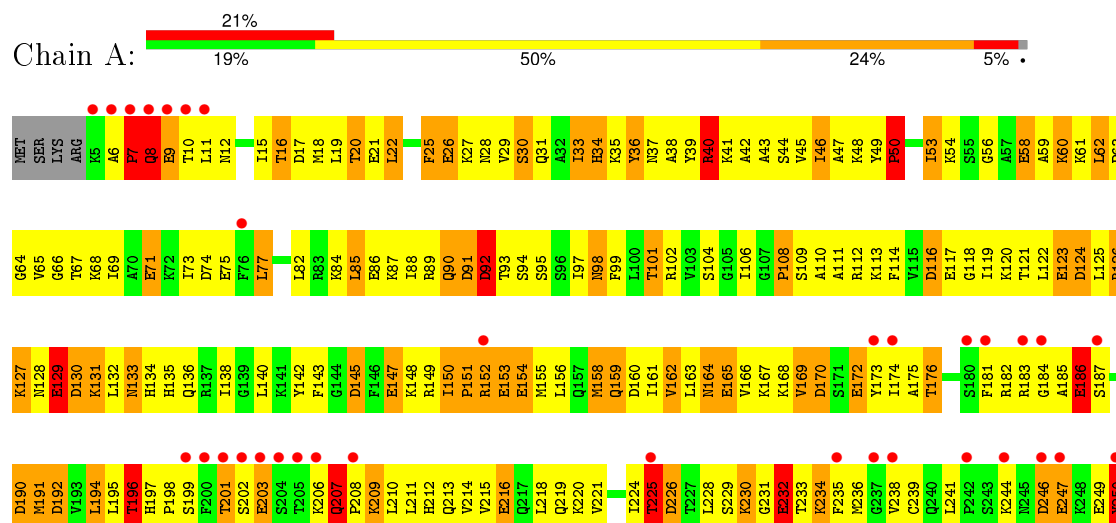
- Molecule 2: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*C)-3')

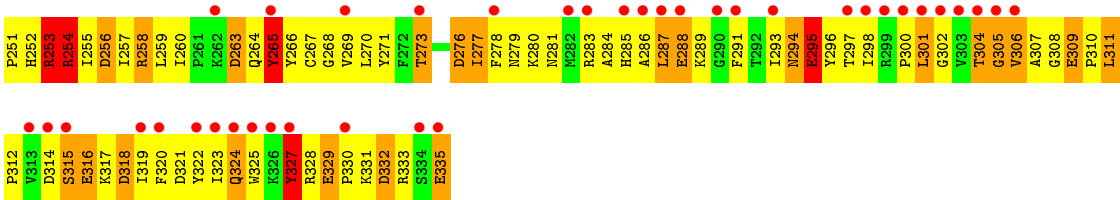


- Molecule 3: DNA (5'-D(\*GP\*TP\*CP\*GP\*G)-3')



- Molecule 4: PROTEIN (DNA POLYMERASE BETA)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.77Å 79.39Å 54.62Å 90.00° 106.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 29.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.40) 96.7 (29.82-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.39Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, $R_{free}$	0.253 , (Not available) 0.251 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 107.9	EDS
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 16520 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	T	2.51	18/362 (5.0%)	2.71	39/556 (7.0%)
2	P	2.35	10/227 (4.4%)	2.65	19/349 (5.4%)
3	D	3.17	12/118 (10.2%)	3.14	17/179 (9.5%)
4	A	1.27	27/2703 (1.0%)	1.69	56/3632 (1.5%)
All	All	1.63	67/3410 (2.0%)	1.99	131/4716 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	1	0

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	4	DA	N3-C4	-15.31	1.25	1.34
1	T	4	DA	C6-N1	-10.72	1.28	1.35
3	D	1	DG	OP3-P	-10.49	1.48	1.61
3	D	1	DG	N7-C5	10.22	1.45	1.39
3	D	5	DG	N9-C4	-8.82	1.30	1.38
3	D	2	DT	C4-C5	-8.54	1.37	1.45
4	A	26	GLU	CD-OE2	8.54	1.35	1.25
4	A	86	GLU	CD-OE2	8.30	1.34	1.25
4	A	117	GLU	CD-OE2	8.25	1.34	1.25
2	P	1	DG	N9-C4	-8.04	1.31	1.38
4	A	186	GLU	CD-OE2	8.03	1.34	1.25
2	P	5	DA	C3'-O3'	-7.96	1.33	1.44
4	A	172	GLU	CD-OE2	7.96	1.34	1.25
3	D	4	DG	N7-C5	7.62	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	7	DG	C5-C6	-7.59	1.34	1.42
4	A	147	GLU	CD-OE2	7.40	1.33	1.25
3	D	5	DG	C5-C6	-7.28	1.35	1.42
1	T	15	DG	N9-C4	-7.19	1.32	1.38
4	A	295	GLU	CD-OE2	6.91	1.33	1.25
4	A	232	GLU	CD-OE2	6.89	1.33	1.25
1	T	7	DG	C6-N1	-6.86	1.34	1.39
2	P	8	DC	C2-O2	-6.82	1.18	1.24
4	A	9	GLU	CB-CG	6.81	1.65	1.52
4	A	71	GLU	CD-OE2	6.80	1.33	1.25
4	A	123	GLU	CD-OE2	6.78	1.33	1.25
2	P	8	DC	N1-C6	-6.74	1.33	1.37
3	D	4	DG	C8-N7	6.64	1.34	1.30
4	A	249	GLU	CD-OE2	6.54	1.32	1.25
3	D	1	DG	N3-C4	-6.52	1.30	1.35
2	P	1	DG	N3-C4	-6.51	1.30	1.35
2	P	9	DG	C3'-O3'	-6.44	1.35	1.44
4	A	153	GLU	CD-OE1	6.43	1.32	1.25
3	D	1	DG	C5-C4	-6.40	1.33	1.38
1	T	16	DC	N1-C2	-6.36	1.33	1.40
1	T	12	DT	P-O5'	-6.28	1.53	1.59
4	A	203	GLU	CD-OE2	6.20	1.32	1.25
4	A	21	GLU	CD-OE2	6.16	1.32	1.25
4	A	216	GLU	CD-OE2	6.10	1.32	1.25
4	A	154	GLU	CD-OE2	6.05	1.32	1.25
4	A	316	GLU	CD-OE2	6.01	1.32	1.25
1	T	1	DC	N1-C6	-5.99	1.33	1.37
3	D	1	DG	C1'-N9	-5.97	1.38	1.47
4	A	58	GLU	CD-OE2	5.96	1.32	1.25
4	A	165	GLU	CD-OE2	5.91	1.32	1.25
2	P	8	DC	C2-N3	-5.80	1.31	1.35
1	T	3	DG	N1-C2	-5.79	1.33	1.37
1	T	3	DG	N7-C5	5.78	1.42	1.39
1	T	4	DA	N7-C5	5.76	1.42	1.39
1	T	3	DG	C5-C6	-5.71	1.36	1.42
1	T	9	DG	N3-C4	-5.59	1.31	1.35
4	A	288	GLU	CD-OE2	5.58	1.31	1.25
4	A	335	GLU	CD-OE2	5.56	1.31	1.25
1	T	2	DC	P-O5'	5.50	1.65	1.59
3	D	3	DC	C5'-C4'	5.49	1.57	1.51
4	A	62	LEU	C-N	-5.39	1.24	1.34
4	A	247	GLU	CD-OE2	5.39	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	9	DG	N1-C2	-5.34	1.33	1.37
4	A	329	GLU	CD-OE2	5.29	1.31	1.25
3	D	1	DG	C8-N7	5.25	1.34	1.30
4	A	75	GLU	CD-OE1	-5.20	1.20	1.25
1	T	9	DG	N1-C2	-5.15	1.33	1.37
2	P	6	DT	C4-C5	-5.14	1.40	1.45
1	T	4	DA	C5-C6	-5.12	1.36	1.41
2	P	8	DC	N3-C4	-5.08	1.30	1.33
4	A	129	GLU	CD-OE2	5.06	1.31	1.25
1	T	2	DC	N1-C2	-5.05	1.35	1.40
1	T	7	DG	N1-C2	-5.02	1.33	1.37

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	150	ILE	C-N-CD	-19.27	78.20	120.60
2	P	7	DG	O4'-C1'-N9	-12.49	99.25	108.00
1	T	2	DC	N3-C4-C5	-11.26	117.39	121.90
3	D	4	DG	C8-N9-C4	10.46	110.58	106.40
1	T	14	DA	O4'-C1'-N9	-10.28	100.81	108.00
1	T	15	DG	C8-N9-C4	10.24	110.50	106.40
3	D	5	DG	N3-C4-C5	10.20	133.70	128.60
2	P	10	DC	P-O5'-C5'	-10.10	104.75	120.90
3	D	1	DG	O4'-C1'-N9	-9.85	101.10	108.00
1	T	8	DC	O4'-C1'-N1	9.73	114.81	108.00
3	D	5	DG	C8-N9-C4	9.65	110.26	106.40
3	D	4	DG	N7-C8-N9	-9.47	108.36	113.10
1	T	1	DC	O4'-C1'-N1	-9.44	101.39	108.00
1	T	7	DG	C8-N9-C4	9.39	110.15	106.40
1	T	12	DT	O4'-C1'-N1	9.34	114.54	108.00
4	A	8	GLN	N-CA-C	8.85	134.89	111.00
4	A	250	TYR	C-N-CD	-8.78	101.28	120.60
3	D	1	DG	C8-N9-C4	8.67	109.87	106.40
2	P	9	DG	C8-N9-C4	8.54	109.82	106.40
1	T	2	DC	C2-N3-C4	8.50	124.15	119.90
4	A	152	ARG	NE-CZ-NH1	8.48	124.54	120.30
4	A	263	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	T	14	DA	C8-N9-C4	8.34	109.14	105.80
4	A	74	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	T	2	DC	P-O3'-C3'	8.06	129.37	119.70
4	A	126	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	T	2	DC	N3-C4-N4	7.83	123.48	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	190	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	T	11	DA	O4'-C1'-N9	-7.74	102.58	108.00
1	T	10	DC	O4'-C1'-N1	7.73	113.41	108.00
4	A	91	ASP	CB-CG-OD2	-7.69	111.38	118.30
2	P	6	DT	N1-C1'-C2'	7.68	127.20	112.60
3	D	5	DG	C2-N3-C4	-7.61	108.09	111.90
4	A	183	ARG	NE-CZ-NH1	7.60	124.10	120.30
3	D	5	DG	N3-C4-N9	-7.59	121.44	126.00
3	D	1	DG	N7-C8-N9	-7.45	109.37	113.10
2	P	4	DG	C8-N9-C4	7.44	109.37	106.40
2	P	2	DC	O4'-C1'-N1	7.38	113.16	108.00
2	P	9	DG	N7-C8-N9	-7.29	109.46	113.10
4	A	17	ASP	CB-CG-OD2	-7.24	111.78	118.30
3	D	2	DT	N1-C1'-C2'	7.22	126.31	112.60
1	T	11	DA	C8-N9-C4	7.16	108.66	105.80
1	T	16	DC	N1-C2-O2	-7.12	114.63	118.90
4	A	130	ASP	CB-CG-OD1	7.03	124.63	118.30
4	A	254	ARG	NE-CZ-NH1	6.98	123.79	120.30
4	A	116	ASP	CB-CG-OD1	6.97	124.58	118.30
3	D	2	DT	C2-N3-C4	-6.96	123.03	127.20
4	A	246	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	T	3	DG	C8-N9-C4	6.81	109.12	106.40
4	A	332	ASP	CB-CG-OD2	-6.76	112.21	118.30
4	A	116	ASP	CB-CG-OD2	-6.70	112.27	118.30
4	A	130	ASP	CB-CG-OD2	-6.64	112.33	118.30
2	P	9	DG	O4'-C1'-N9	-6.63	103.36	108.00
1	T	6	DG	C8-N9-C4	6.61	109.04	106.40
3	D	5	DG	C4-N9-C1'	-6.61	117.91	126.50
4	A	152	ARG	NE-CZ-NH2	-6.59	117.01	120.30
4	A	92	ASP	CB-CG-OD2	-6.56	112.39	118.30
2	P	5	DA	C8-N9-C4	6.55	108.42	105.80
1	T	15	DG	N3-C4-C5	6.50	131.85	128.60
2	P	2	DC	O4'-C1'-C2'	6.48	111.08	105.90
4	A	253	ARG	NE-CZ-NH1	-6.42	117.09	120.30
4	A	246	ASP	CB-CG-OD1	6.41	124.07	118.30
1	T	15	DG	N7-C8-N9	-6.38	109.91	113.10
4	A	318	ASP	CB-CG-OD2	-6.38	112.56	118.30
4	A	60	LYS	N-CA-CB	6.36	122.05	110.60
4	A	124	ASP	CB-CG-OD2	-6.36	112.58	118.30
3	D	5	DG	N7-C8-N9	-6.34	109.93	113.10
4	A	108	PRO	N-CA-CB	6.33	110.89	103.30
4	A	314	ASP	N-CA-CB	6.31	121.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DG	N3-C4-N9	-6.26	122.24	126.00
1	T	13	DC	N1-C1'-C2'	6.25	124.48	112.60
1	T	3	DG	P-O5'-C5'	-6.19	110.99	120.90
1	T	12	DT	P-O3'-C3'	6.15	127.08	119.70
1	T	14	DA	N9-C1'-C2'	6.14	124.28	112.60
2	P	1	DG	N7-C8-N9	-6.08	110.06	113.10
4	A	256	ASP	CB-CG-OD2	-6.07	112.84	118.30
3	D	5	DG	O4'-C1'-C2'	6.06	110.75	105.90
3	D	4	DG	O4'-C1'-N9	5.99	112.20	108.00
4	A	170	ASP	CB-CG-OD1	5.98	123.69	118.30
2	P	1	DG	C8-N9-C4	5.95	108.78	106.40
1	T	10	DC	C2-N1-C1'	-5.92	112.28	118.80
4	A	50	PRO	N-CA-CB	5.92	110.41	103.30
4	A	192	ASP	CB-CG-OD1	5.92	123.63	118.30
1	T	6	DG	O4'-C1'-N9	-5.88	103.88	108.00
4	A	7	PRO	C-N-CA	5.86	136.36	121.70
3	D	4	DG	C4-N9-C1'	-5.86	118.88	126.50
4	A	74	ASP	CB-CG-OD1	5.86	123.57	118.30
4	A	253	ARG	NE-CZ-NH2	5.86	123.23	120.30
4	A	263	ASP	CB-CG-OD1	5.84	123.55	118.30
2	P	5	DA	N9-C1'-C2'	5.79	123.61	112.60
1	T	4	DA	O4'-C1'-N9	-5.79	103.95	108.00
1	T	5	DC	O4'-C1'-N1	5.78	112.04	108.00
1	T	3	DG	O4'-C1'-N9	-5.74	103.98	108.00
4	A	314	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	P	6	DT	C4'-C3'-C2'	5.71	108.24	103.10
1	T	6	DG	N9-C4-C5	-5.69	103.12	105.40
1	T	16	DC	O4'-C1'-C2'	5.69	110.45	105.90
1	T	7	DG	N9-C4-C5	-5.57	103.17	105.40
1	T	7	DG	N7-C8-N9	-5.55	110.32	113.10
4	A	30	SER	N-CA-CB	5.55	118.82	110.50
2	P	7	DG	N9-C1'-C2'	5.53	123.10	112.60
4	A	170	ASP	CB-CG-OD2	-5.51	113.34	118.30
4	A	196	THR	N-CA-CB	5.50	120.75	110.30
2	P	10	DC	O4'-C1'-N1	5.47	111.83	108.00
4	A	196	THR	CA-CB-CG2	5.47	120.06	112.40
4	A	207	GLN	N-CA-CB	5.45	120.41	110.60
3	D	5	DG	N1-C6-O6	5.42	123.15	119.90
1	T	12	DT	OP1-P-OP2	5.35	127.62	119.60
4	A	192	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	T	11	DA	C5-C6-N1	-5.32	115.04	117.70
4	A	314	ASP	CB-CA-C	5.26	120.93	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	14	DA	N9-C4-C5	-5.24	103.70	105.80
4	A	101	THR	CA-CB-CG2	-5.22	105.09	112.40
2	P	1	DG	C4-N9-C1'	-5.20	119.75	126.50
4	A	9	GLU	N-CA-CB	5.20	119.95	110.60
4	A	17	ASP	CB-CG-OD1	5.17	122.95	118.30
4	A	327	TYR	CB-CG-CD1	5.16	124.10	121.00
1	T	13	DC	O4'-C1'-C2'	5.14	110.01	105.90
1	T	11	DA	C6-N1-C2	5.13	121.68	118.60
4	A	89	ARG	NE-CZ-NH1	5.12	122.86	120.30
4	A	145	ASP	CB-CG-OD1	5.12	122.91	118.30
4	A	256	ASP	CB-CG-OD1	5.11	122.89	118.30
1	T	4	DA	N1-C2-N3	5.09	131.84	129.30
4	A	40	ARG	NE-CZ-NH1	5.09	122.84	120.30
4	A	149	ARG	NE-CZ-NH2	-5.07	117.77	120.30
4	A	34	HIS	CA-CB-CG	-5.07	104.99	113.60
4	A	92	ASP	CB-CG-OD1	5.06	122.85	118.30
4	A	332	ASP	CB-CG-OD1	5.05	122.84	118.30
4	A	257	ILE	O-C-N	5.04	130.76	122.70
2	P	9	DG	OP1-P-OP2	-5.01	112.09	119.60
1	T	7	DG	C2-N3-C4	-5.00	109.40	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	314	ASP	CA

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	323	0	179	15	0
2	P	203	0	114	20	0
3	D	106	0	57	10	0
4	A	2653	0	2674	469	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	A	40	0	0	6	0
6	D	6	0	0	1	0
6	P	14	0	0	1	0
6	T	21	0	0	1	0
All	All	3368	0	3024	505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 80.

All (505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:152:ARG:HA	4:A:155:MET:HB2	1.32	1.12
4:A:27:LYS:HE3	4:A:28:ASN:HD21	1.22	1.05
4:A:277:ILE:HG13	4:A:335:GLU:HB3	1.39	1.03
4:A:133:ASN:ND2	4:A:136:GLN:H	1.60	0.97
4:A:33:ILE:H	4:A:33:ILE:HD12	1.29	0.97
2:P:2:DC:H2'	2:P:3:DT:H72	1.46	0.97
4:A:27:LYS:HE3	4:A:28:ASN:ND2	1.84	0.92
4:A:271:TYR:CD2	4:A:295:GLU:HB3	2.06	0.91
4:A:59:ALA:HA	4:A:62:LEU:HD23	1.51	0.91
3:D:2:DT:H4'	4:A:41:LYS:HZ1	1.35	0.91
4:A:301:LEU:HD12	4:A:302:GLY:H	1.37	0.90
4:A:241:LEU:HB2	4:A:250:TYR:CD2	2.09	0.88
2:P:1:DG:H8	2:P:1:DG:H5'	1.39	0.87
4:A:172:GLU:HB3	4:A:198:PRO:CG	2.05	0.87
4:A:133:ASN:H	4:A:136:GLN:HE21	1.22	0.85
4:A:277:ILE:CG1	4:A:335:GLU:HB3	2.07	0.85
4:A:134:HIS:CE1	4:A:138:ILE:HD11	2.13	0.84
4:A:158:MET:HE3	4:A:253:ARG:HH11	1.44	0.83
4:A:197:HIS:CD2	4:A:198:PRO:HD2	2.13	0.83
2:P:1:DG:C8	2:P:1:DG:H5'	2.13	0.83
4:A:286:ALA:HA	4:A:323:ILE:HG21	1.58	0.82
4:A:195:LEU:HD23	4:A:259:LEU:CD1	2.10	0.81
4:A:138:ILE:HD13	4:A:228:LEU:HD13	1.64	0.80
2:P:2:DC:H2'	2:P:3:DT:C7	2.10	0.79
4:A:133:ASN:ND2	4:A:136:GLN:HG3	1.97	0.79
4:A:175:ALA:HB2	4:A:195:LEU:HD12	1.63	0.79
2:P:1:DG:H2'	2:P:2:DC:C6	2.17	0.79
4:A:12:ASN:HD21	4:A:53:ILE:H	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1:DC:H6	1:T:1:DC:HO5'	1.30	0.79
4:A:165:GLU:O	4:A:169:VAL:HG12	1.83	0.79
3:D:2:DT:H4'	4:A:41:LYS:NZ	1.98	0.78
4:A:182:ARG:HE	4:A:273:THR:HG21	1.46	0.77
4:A:37:ASN:HA	4:A:40:ARG:CD	2.13	0.77
4:A:211:LEU:O	4:A:215:VAL:HG23	1.84	0.76
4:A:258:ARG:HB2	4:A:258:ARG:CZ	2.13	0.76
4:A:99:PHE:CD1	4:A:102:ARG:HD3	2.20	0.76
4:A:265:TYR:C	4:A:269:VAL:HG23	2.06	0.76
4:A:265:TYR:O	4:A:269:VAL:HG23	1.86	0.76
4:A:18:MET:HE1	4:A:82:LEU:HD13	1.67	0.76
4:A:210:LEU:O	4:A:214:VAL:HG22	1.85	0.75
4:A:286:ALA:HA	4:A:323:ILE:CG2	2.14	0.75
4:A:34:HIS:HA	6:A:553:HOH:O	1.87	0.75
4:A:131:LYS:O	4:A:132:LEU:HD23	1.86	0.75
4:A:69:ILE:O	4:A:73:ILE:HG13	1.86	0.75
4:A:122:LEU:O	4:A:126:ARG:HG3	1.87	0.74
4:A:15:ILE:O	4:A:19:LEU:HG	1.87	0.74
4:A:18:MET:HE1	4:A:82:LEU:HB2	1.67	0.74
4:A:18:MET:CE	4:A:82:LEU:HD22	2.17	0.74
4:A:159:GLN:O	4:A:163:LEU:HD23	1.88	0.74
4:A:195:LEU:HD23	4:A:259:LEU:HD13	1.69	0.74
4:A:164:ASN:HD22	4:A:164:ASN:N	1.85	0.73
4:A:152:ARG:CA	4:A:155:MET:HB2	2.13	0.73
4:A:182:ARG:NE	4:A:273:THR:HG21	2.03	0.73
4:A:25:PHE:HD2	4:A:88:ILE:HG21	1.54	0.73
4:A:158:MET:CE	4:A:253:ARG:HH11	2.01	0.73
4:A:294:ASN:HD21	4:A:297:THR:H	1.37	0.72
4:A:150:ILE:HD13	4:A:155:MET:HE1	1.71	0.72
4:A:173:TYR:CE1	4:A:210:LEU:HD22	2.23	0.72
4:A:15:ILE:HG21	4:A:46:ILE:HD13	1.71	0.72
4:A:134:HIS:O	4:A:138:ILE:HD12	1.90	0.72
4:A:18:MET:CE	4:A:82:LEU:HD13	2.19	0.71
4:A:158:MET:O	4:A:162:VAL:HG12	1.89	0.71
4:A:150:ILE:HG21	4:A:155:MET:CE	2.19	0.71
3:D:4:DG:H2''	3:D:5:DG:C8	2.25	0.71
4:A:169:VAL:CG2	4:A:213:GLN:HE21	2.03	0.71
4:A:234:LYS:NZ	4:A:234:LYS:HB3	2.05	0.71
4:A:133:ASN:N	4:A:136:GLN:HE21	1.88	0.71
4:A:161:ILE:O	4:A:165:GLU:HG2	1.91	0.71
4:A:281:ASN:O	4:A:284:ALA:HB3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:301:LEU:HD12	4:A:302:GLY:N	2.05	0.70
4:A:288:GLU:CB	4:A:289:LYS:HE3	2.22	0.70
4:A:133:ASN:HD21	4:A:136:GLN:H	1.39	0.70
4:A:172:GLU:HB3	4:A:198:PRO:HG3	1.73	0.69
4:A:59:ALA:HA	4:A:62:LEU:CD2	2.21	0.69
4:A:182:ARG:HE	4:A:273:THR:CG2	2.06	0.69
4:A:154:GLU:OE1	4:A:253:ARG:NH1	2.26	0.69
4:A:194:LEU:CD1	4:A:260:ILE:HD11	2.21	0.69
4:A:37:ASN:HA	4:A:40:ARG:CG	2.23	0.69
4:A:254:ARG:NH1	4:A:254:ARG:HB3	2.07	0.69
2:P:1:DG:H2''	2:P:2:DC:H5'	1.75	0.69
4:A:207:GLN:HB3	4:A:209:LYS:CE	2.22	0.69
4:A:194:LEU:HD11	4:A:260:ILE:HD11	1.75	0.68
4:A:230:LYS:HB3	4:A:230:LYS:NZ	2.07	0.68
2:P:2:DC:H2''	2:P:3:DT:O5'	1.93	0.68
4:A:320:PHE:CD2	4:A:327:TYR:HA	2.28	0.68
4:A:122:LEU:O	4:A:125:LEU:HB2	1.94	0.68
4:A:291:PHE:HD1	4:A:300:PRO:HA	1.59	0.68
4:A:87:LYS:HA	4:A:90:GLN:HG3	1.75	0.68
4:A:266:TYR:HD2	4:A:316:GLU:HG2	1.59	0.67
4:A:172:GLU:HB3	4:A:198:PRO:HG2	1.75	0.67
4:A:152:ARG:O	4:A:156:LEU:N	2.26	0.66
4:A:209:LYS:O	4:A:213:GLN:HB3	1.95	0.66
4:A:161:ILE:HD11	6:A:533:HOH:O	1.95	0.66
4:A:195:LEU:HG	4:A:196:THR:N	2.11	0.66
4:A:267:CYS:SG	4:A:297:THR:HA	2.35	0.66
4:A:25:PHE:CD2	4:A:88:ILE:HG21	2.31	0.66
1:T:4:DA:H2''	1:T:5:DC:O5'	1.96	0.66
4:A:305:GLY:O	4:A:306:VAL:HG13	1.96	0.65
4:A:323:ILE:O	4:A:324:GLN:HG2	1.95	0.65
4:A:293:ILE:HG22	4:A:294:ASN:H	1.61	0.65
4:A:301:LEU:HD11	4:A:306:VAL:HA	1.79	0.65
4:A:328:ARG:NH1	4:A:332:ASP:O	2.29	0.65
4:A:18:MET:HE2	4:A:82:LEU:HD22	1.78	0.65
4:A:152:ARG:NH2	4:A:181:PHE:O	2.29	0.65
4:A:123:GLU:O	4:A:127:LYS:N	2.29	0.65
4:A:278:PHE:CD2	4:A:333:ARG:HB3	2.32	0.65
4:A:33:ILE:HD12	4:A:33:ILE:N	2.08	0.65
4:A:293:ILE:HG22	4:A:294:ASN:N	2.12	0.65
4:A:158:MET:HE1	4:A:253:ARG:HD2	1.79	0.65
3:D:2:DT:H2''	3:D:3:DC:O5'	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:244:LYS:HB3	4:A:247:GLU:HB2	1.79	0.65
4:A:278:PHE:CA	4:A:335:GLU:HA	2.27	0.64
4:A:37:ASN:HA	4:A:40:ARG:HD3	1.78	0.64
4:A:197:HIS:CE1	4:A:199:SER:HB3	2.33	0.64
4:A:285:HIS:NE2	4:A:323:ILE:O	2.29	0.64
4:A:216:GLU:O	4:A:219:GLN:HB2	1.96	0.64
4:A:162:VAL:O	4:A:166:VAL:HG13	1.98	0.64
4:A:166:VAL:O	4:A:169:VAL:HG13	1.98	0.64
4:A:286:ALA:CA	4:A:323:ILE:HG21	2.28	0.64
4:A:131:LYS:C	4:A:132:LEU:HD23	2.18	0.63
4:A:254:ARG:HB3	4:A:254:ARG:HH11	1.63	0.63
4:A:265:TYR:O	4:A:269:VAL:N	2.29	0.63
4:A:145:ASP:O	4:A:148:LYS:HB2	1.99	0.63
1:T:2:DC:H2''	1:T:3:DG:O5'	1.97	0.63
4:A:22:LEU:HD23	4:A:39:TYR:CE1	2.34	0.63
4:A:40:ARG:O	4:A:43:ALA:HB3	1.99	0.63
4:A:28:ASN:HB2	4:A:98:ASN:ND2	2.13	0.62
4:A:197:HIS:CG	4:A:198:PRO:HD2	2.34	0.62
4:A:254:ARG:HH11	4:A:254:ARG:CB	2.12	0.62
4:A:133:ASN:H	4:A:136:GLN:NE2	1.95	0.62
2:P:1:DG:H2''	2:P:2:DC:C5'	2.29	0.62
4:A:236:MET:HE3	4:A:256:ASP:OD2	1.99	0.62
4:A:196:THR:HB	4:A:260:ILE:O	2.00	0.62
4:A:38:ALA:O	4:A:41:LYS:HE2	2.00	0.62
4:A:133:ASN:CG	4:A:136:GLN:HG3	2.20	0.62
4:A:254:ARG:CA	4:A:254:ARG:HH11	2.13	0.62
4:A:309:GLU:CD	4:A:310:PRO:HD2	2.20	0.62
4:A:294:ASN:ND2	4:A:297:THR:H	1.98	0.61
4:A:315:SER:OG	4:A:316:GLU:N	2.29	0.61
4:A:164:ASN:HD22	4:A:164:ASN:H	1.48	0.61
4:A:90:GLN:HE21	4:A:91:ASP:N	1.98	0.61
4:A:138:ILE:HD13	4:A:228:LEU:CD1	2.31	0.61
4:A:128:ASN:HB3	4:A:131:LYS:CG	2.31	0.61
4:A:28:ASN:O	4:A:108:PRO:HB3	2.00	0.61
4:A:317:LYS:HD3	4:A:327:TYR:HD2	1.65	0.61
4:A:56:GLY:O	4:A:60:LYS:N	2.32	0.61
4:A:41:LYS:NZ	6:A:563:HOH:O	2.30	0.61
4:A:87:LYS:HA	4:A:90:GLN:CG	2.30	0.61
4:A:271:TYR:HD2	4:A:295:GLU:HB3	1.62	0.61
4:A:67:THR:O	4:A:71:GLU:HG3	2.01	0.61
1:T:10:DC:O3'	4:A:229:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:166:VAL:HA	4:A:169:VAL:CG1	2.31	0.61
4:A:7:PRO:O	4:A:8:GLN:HG2	1.99	0.60
4:A:128:ASN:O	4:A:130:ASP:N	2.33	0.60
4:A:169:VAL:HG22	4:A:213:GLN:HE21	1.64	0.60
4:A:165:GLU:O	4:A:168:LYS:HB2	2.01	0.60
4:A:128:ASN:HB3	4:A:131:LYS:HG3	1.83	0.60
4:A:8:GLN:HB3	4:A:47:ALA:O	2.00	0.60
4:A:7:PRO:C	4:A:8:GLN:HG2	2.22	0.60
4:A:119:ILE:HG23	4:A:124:ASP:HB2	1.83	0.60
4:A:196:THR:HG23	4:A:265:TYR:CD1	2.37	0.60
4:A:153:GLU:OE2	4:A:153:GLU:HA	2.01	0.60
4:A:298:ILE:HD13	4:A:322:TYR:HD2	1.67	0.60
4:A:150:ILE:CD1	4:A:155:MET:HE1	2.31	0.60
4:A:175:ALA:HB2	4:A:195:LEU:CD1	2.31	0.60
1:T:1:DC:H2''	1:T:2:DC:O5'	2.01	0.60
4:A:133:ASN:HD22	4:A:135:HIS:N	2.00	0.60
4:A:207:GLN:HB3	4:A:209:LYS:HD3	1.84	0.60
4:A:266:TYR:CD2	4:A:316:GLU:HG2	2.37	0.60
4:A:99:PHE:HD1	4:A:102:ARG:HD3	1.67	0.60
4:A:102:ARG:HH21	4:A:147:GLU:CD	2.04	0.60
4:A:196:THR:HG22	4:A:260:ILE:HB	1.83	0.59
4:A:42:ALA:O	4:A:46:ILE:HG23	2.01	0.59
4:A:59:ALA:CA	4:A:62:LEU:HD23	2.29	0.59
4:A:232:GLU:CD	4:A:233:THR:HG23	2.23	0.59
4:A:163:LEU:O	4:A:166:VAL:HG22	2.01	0.59
4:A:132:LEU:HB3	4:A:136:GLN:HB2	1.85	0.59
4:A:155:MET:O	4:A:159:GLN:HB3	2.02	0.59
4:A:156:LEU:O	4:A:159:GLN:HG2	2.03	0.59
4:A:207:GLN:HG3	4:A:210:LEU:CD1	2.32	0.59
4:A:169:VAL:HG21	4:A:213:GLN:CG	2.33	0.58
4:A:317:LYS:O	4:A:320:PHE:N	2.36	0.58
4:A:152:ARG:HH21	4:A:185:ALA:N	2.01	0.58
4:A:26:GLU:O	4:A:31:GLN:N	2.35	0.58
4:A:278:PHE:HA	4:A:335:GLU:HA	1.86	0.58
4:A:62:LEU:HB2	4:A:65:VAL:CG2	2.34	0.58
4:A:164:ASN:N	4:A:164:ASN:ND2	2.52	0.58
4:A:135:HIS:HA	4:A:228:LEU:HD12	1.84	0.58
4:A:302:GLY:CA	4:A:307:ALA:HB3	2.33	0.58
4:A:289:LYS:HB3	4:A:324:GLN:OE1	2.03	0.58
4:A:104:SER:OG	4:A:135:HIS:HE1	1.87	0.58
4:A:254:ARG:NH1	4:A:255:ILE:N	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:288:GLU:HB3	4:A:289:LYS:HE3	1.86	0.57
4:A:138:ILE:HG22	4:A:142:TYR:HD2	1.70	0.57
4:A:165:GLU:HA	4:A:168:LYS:HD2	1.86	0.57
4:A:254:ARG:HH11	4:A:255:ILE:N	2.01	0.57
4:A:195:LEU:HD23	4:A:259:LEU:HD12	1.86	0.57
4:A:158:MET:HE3	4:A:253:ARG:NH1	2.15	0.57
4:A:176:THR:HG22	4:A:265:TYR:OH	2.05	0.57
4:A:142:TYR:HE1	4:A:252:HIS:CE1	2.23	0.56
4:A:320:PHE:CG	4:A:327:TYR:HA	2.40	0.56
4:A:151:PRO:O	4:A:155:MET:N	2.30	0.56
4:A:192:ASP:CG	4:A:258:ARG:HH22	2.08	0.56
4:A:150:ILE:HG21	4:A:155:MET:HE2	1.87	0.56
4:A:152:ARG:HA	4:A:155:MET:CB	2.22	0.56
4:A:302:GLY:HA2	4:A:307:ALA:HB3	1.87	0.56
4:A:285:HIS:O	4:A:288:GLU:N	2.39	0.56
4:A:208:PRO:HD2	4:A:209:LYS:HD2	1.85	0.56
4:A:224:ILE:HA	4:A:239:CYS:HA	1.88	0.56
4:A:317:LYS:O	4:A:320:PHE:HB2	2.05	0.56
4:A:173:TYR:OH	4:A:210:LEU:HD23	2.06	0.56
4:A:44:SER:O	4:A:47:ALA:HB3	2.06	0.56
4:A:124:ASP:O	4:A:128:ASN:ND2	2.28	0.56
4:A:154:GLU:O	4:A:158:MET:N	2.28	0.56
4:A:266:TYR:HA	4:A:269:VAL:CG2	2.36	0.56
4:A:267:CYS:HB3	4:A:295:GLU:O	2.06	0.55
4:A:291:PHE:CD1	4:A:300:PRO:HA	2.41	0.55
4:A:316:GLU:O	4:A:319:ILE:HB	2.07	0.55
4:A:239:CYS:HB3	4:A:255:ILE:HG21	1.88	0.55
4:A:278:PHE:CE2	4:A:333:ARG:HG2	2.41	0.55
4:A:99:PHE:CE1	4:A:143:PHE:HZ	2.25	0.55
4:A:234:LYS:HZ3	4:A:234:LYS:HB3	1.71	0.55
4:A:152:ARG:O	4:A:156:LEU:HG	2.07	0.55
4:A:62:LEU:HB2	4:A:65:VAL:HG21	1.88	0.55
2:P:1:DG:H2'	2:P:2:DC:C5	2.41	0.55
4:A:25:PHE:CE2	4:A:88:ILE:HD13	2.42	0.55
4:A:295:GLU:HG2	4:A:296:TYR:CE2	2.43	0.54
4:A:201:THR:HG23	4:A:202:SER:N	2.22	0.54
4:A:221:VAL:HG22	4:A:221:VAL:O	2.07	0.54
4:A:93:THR:O	4:A:97:ILE:HG13	2.07	0.54
4:A:134:HIS:HB3	6:A:523:HOH:O	2.07	0.54
4:A:145:ASP:OD2	4:A:252:HIS:N	2.29	0.54
4:A:132:LEU:HA	4:A:136:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:150:ILE:HG12	4:A:253:ARG:CZ	2.38	0.54
4:A:207:GLN:HG3	4:A:210:LEU:HD11	1.90	0.54
4:A:254:ARG:NH1	4:A:255:ILE:H	2.06	0.54
4:A:241:LEU:HB2	4:A:250:TYR:CE2	2.43	0.54
4:A:18:MET:CE	4:A:82:LEU:HB2	2.36	0.54
4:A:33:ILE:H	4:A:33:ILE:CD1	2.11	0.54
3:D:1:DG:H2'	3:D:2:DT:H71	1.89	0.54
4:A:241:LEU:HB2	4:A:250:TYR:HD2	1.70	0.54
4:A:150:ILE:CG2	4:A:155:MET:HE2	2.37	0.54
4:A:207:GLN:O	4:A:210:LEU:HB2	2.06	0.54
4:A:324:GLN:O	4:A:325:TRP:HD1	1.90	0.54
4:A:53:ILE:HG22	4:A:54:LYS:N	2.23	0.54
4:A:279:ASN:O	4:A:283:ARG:HG3	2.08	0.53
4:A:25:PHE:HE2	4:A:88:ILE:HG12	1.73	0.53
4:A:138:ILE:HG23	4:A:142:TYR:CE2	2.43	0.53
4:A:150:ILE:HG21	4:A:155:MET:HE1	1.90	0.53
4:A:169:VAL:HG11	4:A:214:VAL:HG12	1.90	0.53
3:D:2:DT:C4'	4:A:41:LYS:HZ1	2.16	0.53
4:A:207:GLN:CB	4:A:209:LYS:HD3	2.37	0.53
4:A:192:ASP:OD1	4:A:258:ARG:NH2	2.41	0.53
4:A:265:TYR:O	4:A:268:GLY:N	2.40	0.53
1:T:2:DC:H2''	1:T:3:DG:C8	2.44	0.53
4:A:288:GLU:C	4:A:289:LYS:HE3	2.29	0.53
4:A:37:ASN:C	4:A:40:ARG:HG2	2.29	0.53
4:A:232:GLU:OE2	4:A:233:THR:HG23	2.09	0.53
1:T:9:DG:N7	6:T:530:HOH:O	2.33	0.53
3:D:1:DG:N7	6:D:536:HOH:O	2.34	0.53
4:A:15:ILE:HG21	4:A:46:ILE:CD1	2.38	0.53
4:A:119:ILE:HG23	4:A:124:ASP:CB	2.39	0.52
4:A:216:GLU:O	4:A:220:LYS:N	2.32	0.52
4:A:196:THR:OG1	4:A:197:HIS:N	2.41	0.52
2:P:4:DG:C2	2:P:5:DA:C5	2.98	0.52
4:A:287:LEU:HD22	4:A:291:PHE:O	2.09	0.52
4:A:174:ILE:O	4:A:195:LEU:HD12	2.09	0.52
4:A:26:GLU:HA	4:A:30:SER:HB2	1.92	0.52
4:A:182:ARG:HB3	4:A:273:THR:CG2	2.40	0.52
4:A:48:LYS:O	4:A:50:PRO:HD3	2.10	0.52
4:A:155:MET:O	4:A:159:GLN:N	2.43	0.52
4:A:207:GLN:HB3	4:A:209:LYS:CD	2.40	0.52
4:A:186:GLU:N	4:A:186:GLU:OE1	2.43	0.52
4:A:112:ARG:HD2	6:A:517:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:164:ASN:O	4:A:167:LYS:HB3	2.10	0.52
4:A:269:VAL:O	4:A:273:THR:OG1	2.26	0.52
4:A:301:LEU:CD1	4:A:306:VAL:HA	2.40	0.52
4:A:73:ILE:O	4:A:77:LEU:HD22	2.10	0.51
4:A:202:SER:OG	4:A:263:ASP:OD2	2.25	0.51
4:A:311:LEU:N	4:A:311:LEU:HD13	2.25	0.51
4:A:295:GLU:HG2	4:A:296:TYR:CD2	2.45	0.51
4:A:331:LYS:O	4:A:331:LYS:HD2	2.09	0.51
4:A:315:SER:OG	4:A:317:LYS:N	2.41	0.51
4:A:286:ALA:CB	4:A:323:ILE:HG21	2.40	0.51
1:T:10:DC:H5'	4:A:234:LYS:HZ3	1.75	0.51
4:A:142:TYR:CE1	4:A:252:HIS:CE1	2.99	0.51
4:A:175:ALA:HA	4:A:194:LEU:O	2.10	0.51
4:A:194:LEU:HD12	4:A:260:ILE:CD1	2.41	0.51
4:A:191:MET:HG2	4:A:255:ILE:HG13	1.92	0.51
4:A:87:LYS:CA	4:A:90:GLN:HG3	2.41	0.51
4:A:194:LEU:HD12	4:A:260:ILE:HD11	1.91	0.50
4:A:298:ILE:HD13	4:A:322:TYR:CD2	2.46	0.50
4:A:304:THR:OG1	4:A:305:GLY:N	2.45	0.50
4:A:285:HIS:CG	4:A:325:TRP:NE1	2.80	0.50
4:A:84:LYS:HG2	4:A:88:ILE:CD1	2.41	0.50
4:A:138:ILE:HG22	4:A:142:TYR:CD2	2.47	0.50
4:A:288:GLU:N	4:A:288:GLU:OE2	2.44	0.50
1:T:1:DC:H6	1:T:1:DC:O5'	1.90	0.50
2:P:9:DG:H2''	2:P:10:DC:O5'	2.11	0.50
4:A:142:TYR:CE1	4:A:252:HIS:ND1	2.80	0.50
4:A:197:HIS:CE1	4:A:199:SER:H	2.27	0.50
2:P:4:DG:N7	6:P:506:HOH:O	2.33	0.50
4:A:312:PRO:O	4:A:322:TYR:OH	2.30	0.50
4:A:12:ASN:O	4:A:16:THR:OG1	2.30	0.50
2:P:4:DG:C4	2:P:5:DA:N7	2.80	0.50
4:A:285:HIS:CE1	4:A:325:TRP:NE1	2.79	0.50
4:A:91:ASP:O	4:A:94:SER:OG	2.29	0.50
4:A:207:GLN:HB3	4:A:209:LYS:HE2	1.93	0.50
4:A:318:ASP:HA	4:A:321:ASP:HB2	1.94	0.50
4:A:250:TYR:HB3	4:A:251:PRO:CD	2.42	0.50
4:A:16:THR:O	4:A:20:THR:OG1	2.30	0.50
4:A:126:ARG:O	4:A:129:GLU:OE1	2.30	0.49
4:A:12:ASN:HD21	4:A:53:ILE:N	2.04	0.49
4:A:19:LEU:O	4:A:22:LEU:HB2	2.12	0.49
4:A:287:LEU:HB3	4:A:288:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:37:ASN:CA	4:A:40:ARG:HG2	2.42	0.49
4:A:36:TYR:O	4:A:40:ARG:HG2	2.12	0.49
4:A:58:GLU:O	4:A:61:LYS:HB3	2.12	0.49
4:A:154:GLU:O	4:A:158:MET:HG3	2.13	0.49
4:A:116:ASP:C	4:A:118:GLY:H	2.16	0.49
4:A:110:ALA:O	4:A:113:LYS:HB3	2.13	0.49
4:A:150:ILE:HG22	4:A:151:PRO:N	2.27	0.49
4:A:151:PRO:O	4:A:154:GLU:N	2.45	0.49
4:A:28:ASN:HA	4:A:108:PRO:HG3	1.94	0.49
4:A:82:LEU:O	4:A:85:LEU:N	2.46	0.49
4:A:15:ILE:O	4:A:18:MET:HG2	2.13	0.48
4:A:84:LYS:HG2	4:A:88:ILE:HD12	1.95	0.48
4:A:97:ILE:O	4:A:101:THR:HG23	2.13	0.48
2:P:7:DG:H2''	2:P:8:DC:O5'	2.13	0.48
4:A:173:TYR:OH	4:A:210:LEU:O	2.29	0.48
4:A:169:VAL:HG21	4:A:213:GLN:HG3	1.95	0.48
4:A:278:PHE:CE2	4:A:333:ARG:HB3	2.48	0.48
4:A:68:LYS:HA	4:A:71:GLU:HG3	1.96	0.48
4:A:99:PHE:CZ	4:A:143:PHE:CZ	3.01	0.48
4:A:196:THR:CG2	4:A:265:TYR:CD1	2.96	0.48
4:A:285:HIS:CE1	4:A:325:TRP:HE1	2.32	0.48
4:A:234:LYS:HZ2	4:A:234:LYS:HB3	1.76	0.48
4:A:62:LEU:HA	4:A:63:PRO:HD3	1.67	0.48
4:A:37:ASN:HA	4:A:40:ARG:HG2	1.95	0.48
4:A:150:ILE:HG12	4:A:253:ARG:NE	2.29	0.48
4:A:152:ARG:NH2	4:A:184:GLY:CA	2.77	0.47
4:A:65:VAL:HG12	4:A:66:GLY:N	2.28	0.47
4:A:122:LEU:HA	4:A:122:LEU:HD23	1.81	0.47
4:A:138:ILE:HG21	4:A:238:VAL:HG21	1.96	0.47
4:A:192:ASP:OD1	4:A:258:ARG:NH1	2.46	0.47
4:A:35:LYS:O	4:A:39:TYR:HD2	1.97	0.47
4:A:317:LYS:O	4:A:321:ASP:N	2.41	0.47
1:T:3:DG:H2''	1:T:4:DA:O5'	2.14	0.47
4:A:175:ALA:C	4:A:176:THR:HG22	2.35	0.47
4:A:9:GLU:C	4:A:11:LEU:H	2.18	0.47
4:A:18:MET:HE2	4:A:82:LEU:HD13	1.96	0.47
4:A:224:ILE:HG23	4:A:238:VAL:O	2.14	0.47
4:A:158:MET:CE	4:A:253:ARG:HD2	2.42	0.47
4:A:287:LEU:HA	4:A:291:PHE:O	2.14	0.47
4:A:155:MET:HE3	4:A:190:ASP:O	2.15	0.47
4:A:209:LYS:O	4:A:212:HIS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:41:LYS:HE3	4:A:64:GLY:O	2.15	0.47
4:A:150:ILE:CG2	4:A:151:PRO:N	2.78	0.46
4:A:150:ILE:HG22	4:A:155:MET:HG2	1.96	0.46
4:A:236:MET:HB3	4:A:256:ASP:OD2	2.14	0.46
4:A:216:GLU:HA	4:A:219:GLN:HB2	1.96	0.46
4:A:114:PHE:HZ	4:A:132:LEU:HD22	1.80	0.46
4:A:197:HIS:CG	4:A:198:PRO:CD	2.98	0.46
4:A:285:HIS:ND1	4:A:325:TRP:NE1	2.63	0.46
1:T:15:DG:H2''	1:T:16:DC:C6	2.50	0.46
4:A:114:PHE:CZ	4:A:132:LEU:HD22	2.51	0.46
4:A:317:LYS:HD3	4:A:327:TYR:CD2	2.49	0.46
4:A:151:PRO:O	4:A:154:GLU:HB2	2.15	0.46
4:A:285:HIS:HD2	4:A:323:ILE:HD12	1.80	0.46
4:A:228:LEU:HA	4:A:228:LEU:HD13	1.81	0.46
2:P:4:DG:H2''	2:P:5:DA:H8	1.80	0.46
4:A:25:PHE:CE2	4:A:88:ILE:CD1	2.98	0.46
4:A:234:LYS:HG2	4:A:235:PHE:N	2.31	0.46
4:A:186:GLU:OE1	4:A:187:SER:N	2.48	0.46
4:A:166:VAL:CG2	4:A:167:LYS:N	2.79	0.46
1:T:2:DC:C2'	1:T:3:DG:C8	2.99	0.46
4:A:25:PHE:CE2	4:A:88:ILE:HG12	2.51	0.46
4:A:278:PHE:CE2	4:A:333:ARG:CG	2.99	0.45
4:A:133:ASN:ND2	4:A:136:GLN:N	2.45	0.45
4:A:225:THR:OG1	4:A:226:ASP:OD1	2.31	0.45
4:A:278:PHE:CE2	4:A:333:ARG:CB	2.99	0.45
3:D:2:DT:H4'	4:A:64:GLY:O	2.16	0.45
4:A:62:LEU:HB3	4:A:63:PRO:HD2	1.98	0.45
4:A:45:VAL:HG23	4:A:46:ILE:N	2.31	0.45
1:T:10:DC:H5'	4:A:234:LYS:NZ	2.31	0.45
4:A:230:LYS:HB3	4:A:230:LYS:HZ1	1.78	0.45
4:A:138:ILE:CG2	4:A:142:TYR:CD2	3.00	0.45
4:A:152:ARG:NH2	4:A:184:GLY:HA2	2.32	0.45
4:A:196:THR:HG23	4:A:265:TYR:CE1	2.51	0.45
2:P:3:DT:C2'	2:P:4:DG:C8	2.99	0.45
4:A:60:LYS:HG3	4:A:66:GLY:HA2	1.98	0.45
4:A:288:GLU:HA	4:A:288:GLU:OE1	2.07	0.45
3:D:1:DG:OP2	4:A:68:LYS:HE2	2.17	0.45
4:A:37:ASN:O	4:A:40:ARG:HG2	2.16	0.45
4:A:159:GLN:CG	4:A:160:ASP:N	2.79	0.45
4:A:298:ILE:HG23	4:A:298:ILE:O	2.17	0.45
4:A:85:LEU:HD12	4:A:85:LEU:HA	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:278:PHE:HB2	4:A:335:GLU:HA	1.99	0.45
4:A:125:LEU:HB3	4:A:140:LEU:HD22	1.98	0.45
4:A:197:HIS:HE1	4:A:199:SER:HB3	1.81	0.45
4:A:192:ASP:CG	4:A:258:ARG:HH12	2.20	0.45
4:A:250:TYR:HB3	4:A:251:PRO:HD2	1.99	0.45
4:A:18:MET:HE3	4:A:18:MET:HB2	1.86	0.45
4:A:285:HIS:CB	4:A:325:TRP:CZ2	3.00	0.44
4:A:276:ASP:O	4:A:280:LYS:HG3	2.17	0.44
4:A:142:TYR:CE1	4:A:252:HIS:CG	3.05	0.44
4:A:270:LEU:HD22	4:A:319:ILE:HG21	1.98	0.44
4:A:62:LEU:CB	4:A:63:PRO:HD2	2.46	0.44
4:A:195:LEU:HG	4:A:196:THR:H	1.78	0.44
4:A:28:ASN:CB	4:A:98:ASN:ND2	2.80	0.44
4:A:194:LEU:HD21	4:A:258:ARG:NH1	2.32	0.44
4:A:77:LEU:HD13	4:A:77:LEU:HA	1.87	0.44
4:A:309:GLU:OE1	4:A:309:GLU:HA	2.16	0.44
4:A:125:LEU:HD23	4:A:125:LEU:HA	1.71	0.44
4:A:255:ILE:HG12	4:A:256:ASP:N	2.33	0.44
3:D:4:DG:H2"	3:D:5:DG:N7	2.32	0.44
4:A:194:LEU:O	4:A:265:TYR:OH	2.29	0.44
4:A:169:VAL:CG2	4:A:213:GLN:NE2	2.77	0.44
4:A:254:ARG:HH11	4:A:255:ILE:H	1.64	0.44
4:A:285:HIS:CG	4:A:325:TRP:CE2	3.06	0.44
4:A:25:PHE:CD2	4:A:88:ILE:HD13	2.52	0.44
1:T:2:DC:H2"	1:T:3:DG:H8	1.83	0.44
4:A:128:ASN:C	4:A:130:ASP:H	2.21	0.43
4:A:138:ILE:CG2	4:A:142:TYR:CE2	3.01	0.43
4:A:159:GLN:HG2	4:A:160:ASP:N	2.32	0.43
4:A:208:PRO:O	4:A:212:HIS:HB2	2.17	0.43
4:A:211:LEU:O	4:A:214:VAL:HG23	2.18	0.43
4:A:197:HIS:ND1	4:A:199:SER:CB	2.80	0.43
4:A:99:PHE:O	4:A:102:ARG:HG3	2.18	0.43
4:A:266:TYR:HD1	6:A:574:HOH:O	2.01	0.43
4:A:121:THR:OG1	4:A:123:GLU:HB2	2.18	0.43
4:A:25:PHE:CD2	4:A:88:ILE:CG2	3.00	0.43
4:A:216:GLU:C	4:A:219:GLN:HB2	2.38	0.43
4:A:133:ASN:HD21	4:A:135:HIS:HB3	1.83	0.43
4:A:163:LEU:HA	4:A:163:LEU:HD13	1.77	0.43
4:A:163:LEU:N	4:A:163:LEU:HD22	2.34	0.43
4:A:106:ILE:CG2	4:A:111:ALA:HB2	2.49	0.43
4:A:190:ASP:OD1	4:A:190:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:11:DA:C5'	4:A:229:SER:HB3	2.49	0.43
4:A:28:ASN:HB2	4:A:98:ASN:HD21	1.84	0.43
4:A:327:TYR:CE1	4:A:333:ARG:NH2	2.87	0.43
2:P:4:DG:C2	2:P:5:DA:C4	3.07	0.43
4:A:211:LEU:HD23	4:A:231:GLY:O	2.19	0.42
4:A:135:HIS:CG	4:A:228:LEU:HD12	2.54	0.42
4:A:132:LEU:CA	4:A:136:GLN:HE21	2.32	0.42
4:A:173:TYR:HE1	4:A:210:LEU:HD22	1.77	0.42
4:A:22:LEU:HA	4:A:22:LEU:HD12	1.73	0.42
4:A:11:LEU:HA	4:A:11:LEU:HD23	1.78	0.42
4:A:133:ASN:HD22	4:A:133:ASN:C	2.22	0.42
4:A:301:LEU:HD12	4:A:301:LEU:HA	1.59	0.42
4:A:150:ILE:CD1	4:A:155:MET:CE	2.97	0.42
4:A:225:THR:OG1	4:A:226:ASP:N	2.52	0.42
4:A:278:PHE:CD2	4:A:333:ARG:CB	3.00	0.42
4:A:293:ILE:CD1	4:A:298:ILE:HD12	2.49	0.42
4:A:317:LYS:CD	4:A:327:TYR:HB2	2.49	0.42
4:A:45:VAL:CG2	4:A:46:ILE:N	2.81	0.42
4:A:166:VAL:O	4:A:170:ASP:O	2.37	0.42
4:A:194:LEU:HA	4:A:194:LEU:HD13	1.14	0.42
4:A:133:ASN:ND2	4:A:135:HIS:N	2.66	0.42
4:A:53:ILE:CG2	4:A:54:LYS:N	2.83	0.42
4:A:6:ALA:HA	4:A:7:PRO:HD3	1.60	0.42
4:A:329:GLU:O	4:A:333:ARG:HG3	2.20	0.42
2:P:4:DG:H2''	2:P:5:DA:OP2	2.19	0.42
4:A:164:ASN:O	4:A:167:LYS:N	2.53	0.41
4:A:293:ILE:CG2	4:A:294:ASN:N	2.81	0.41
4:A:285:HIS:HB2	4:A:325:TRP:CZ2	2.56	0.41
4:A:285:HIS:CE1	4:A:289:LYS:NZ	2.88	0.41
4:A:234:LYS:CG	4:A:235:PHE:N	2.83	0.41
4:A:133:ASN:HD21	4:A:136:GLN:N	2.13	0.41
4:A:142:TYR:OH	4:A:226:ASP:OD1	2.26	0.41
4:A:228:LEU:HD22	4:A:228:LEU:N	2.35	0.41
4:A:68:LYS:O	4:A:71:GLU:HB2	2.20	0.41
4:A:73:ILE:HG22	4:A:73:ILE:O	2.20	0.41
4:A:165:GLU:HG3	4:A:218:LEU:HD23	2.02	0.41
4:A:252:HIS:C	4:A:253:ARG:HG2	2.37	0.41
4:A:254:ARG:NH1	4:A:256:ASP:OD1	2.51	0.41
4:A:166:VAL:CA	4:A:169:VAL:CG1	2.99	0.41
4:A:19:LEU:HD12	4:A:43:ALA:HA	2.01	0.41
4:A:289:LYS:HD3	4:A:289:LYS:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:49:TYR:HE1	4:A:53:ILE:HG12	1.85	0.41
4:A:254:ARG:NH1	4:A:254:ARG:CB	2.77	0.41
4:A:73:ILE:HG22	4:A:77:LEU:CD2	2.51	0.41
4:A:316:GLU:HB2	4:A:327:TYR:CZ	2.56	0.41
4:A:138:ILE:HG23	4:A:142:TYR:HE2	1.83	0.41
4:A:132:LEU:CA	4:A:136:GLN:NE2	2.84	0.41
4:A:266:TYR:HA	4:A:269:VAL:HG23	2.02	0.41
4:A:330:PRO:HA	4:A:333:ARG:CD	2.51	0.41
2:P:3:DT:H2''	2:P:4:DG:O5'	2.20	0.41
2:P:5:DA:H2''	2:P:6:DT:OP2	2.21	0.41
4:A:267:CYS:SG	4:A:296:TYR:O	2.79	0.41
4:A:216:GLU:CA	4:A:219:GLN:HB2	2.50	0.41
4:A:254:ARG:HD2	4:A:254:ARG:HA	1.90	0.41
4:A:317:LYS:HD3	4:A:327:TYR:HB2	2.03	0.41
4:A:241:LEU:CB	4:A:250:TYR:CE2	3.03	0.41
4:A:90:GLN:HE21	4:A:91:ASP:CA	2.34	0.41
4:A:18:MET:HE3	4:A:82:LEU:HD22	1.97	0.40
4:A:25:PHE:O	4:A:29:VAL:HB	2.21	0.40
4:A:110:ALA:HA	4:A:113:LYS:HE2	2.03	0.40
4:A:129:GLU:HA	4:A:132:LEU:HG	2.04	0.40
4:A:49:TYR:CE1	4:A:53:ILE:HG12	2.57	0.40
4:A:15:ILE:CG2	4:A:46:ILE:CD1	2.99	0.40
4:A:197:HIS:CG	4:A:198:PRO:N	2.90	0.40
4:A:293:ILE:HD11	4:A:298:ILE:HD12	2.02	0.40
4:A:166:VAL:HG23	4:A:167:LYS:N	2.36	0.40
4:A:92:ASP:HB2	4:A:93:THR:H	1.73	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	329/335 (98%)	268 (82%)	47 (14%)	14 (4%)	3 2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	7	PRO
4	A	8	GLN
4	A	129	GLU
4	A	250	TYR
4	A	92	ASP
4	A	232	GLU
4	A	308	GLY
4	A	50	PRO
4	A	265	TYR
4	A	305	GLY
4	A	225	THR
4	A	309	GLU
4	A	306	VAL
4	A	53	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	291/295 (99%)	233 (80%)	58 (20%)	1 2

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	THR
4	A	16	THR
4	A	20	THR
4	A	22	LEU
4	A	25	PHE
4	A	33	ILE
4	A	36	TYR

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Mol	Chain	Res	Type
4	A	40	ARG
4	A	46	ILE
4	A	77	LEU
4	A	85	LEU
4	A	90	GLN
4	A	95	SER
4	A	98	ASN
4	A	109	SER
4	A	120	LYS
4	A	127	LYS
4	A	131	LYS
4	A	133	ASN
4	A	151	PRO
4	A	158	MET
4	A	159	GLN
4	A	162	VAL
4	A	164	ASN
4	A	169	VAL
4	A	176	THR
4	A	186	GLU
4	A	191	MET
4	A	194	LEU
4	A	196	THR
4	A	201	THR
4	A	203	GLU
4	A	206	LYS
4	A	207	GLN
4	A	209	LYS
4	A	225	THR
4	A	226	ASP
4	A	230	LYS
4	A	232	GLU
4	A	234	LYS
4	A	246	ASP
4	A	253	ARG
4	A	254	ARG
4	A	258	ARG
4	A	264	GLN
4	A	265	TYR
4	A	273	THR
4	A	276	ASP
4	A	277	ILE

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Mol	Chain	Res	Type
4	A	287	LEU
4	A	294	ASN
4	A	295	GLU
4	A	301	LEU
4	A	304	THR
4	A	311	LEU
4	A	315	SER
4	A	324	GLN
4	A	327	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	8	GLN
4	A	12	ASN
4	A	28	ASN
4	A	90	GLN
4	A	98	ASN
4	A	133	ASN
4	A	135	HIS
4	A	136	GLN
4	A	159	GLN
4	A	164	ASN
4	A	212	HIS
4	A	213	GLN
4	A	217	GLN
4	A	245	ASN
4	A	281	ASN
4	A	294	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	T	16/16 (100%)	0.69	1 (6%) 23 24	42, 56, 69, 71	0
2	P	10/10 (100%)	0.79	1 (10%) 9 9	45, 54, 72, 73	0
3	D	5/5 (100%)	-0.17	0 100 100	32, 40, 48, 49	0
4	A	331/335 (98%)	1.23	72 (21%) 1 1	24, 60, 99, 100	75 (22%)
All	All	362/366 (98%)	1.18	74 (20%) 1 1	24, 60, 99, 100	75 (20%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	208	PRO	7.8
4	A	204	SER	6.7
4	A	8	GLN	6.6
4	A	287	LEU	6.3
4	A	205	THR	5.4
4	A	288	GLU	5.0
4	A	313	VAL	4.9
4	A	303	VAL	4.8
4	A	184	GLY	4.6
4	A	265	TYR	4.5
4	A	301	LEU	4.2
4	A	5	LYS	4.1
4	A	244	LYS	4.1
4	A	324	GLN	3.9
4	A	322	TYR	3.8
4	A	326	LYS	3.8
4	A	330	PRO	3.8
4	A	203	GLU	3.8
4	A	246	ASP	3.7
4	A	201	THR	3.6
4	A	180	SER	3.5

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Mol	Chain	Res	Type	RSRZ
4	A	305	GLY	3.5
4	A	327	TYR	3.5
4	A	9	GLU	3.5
4	A	300	PRO	3.4
4	A	285	HIS	3.3
4	A	286	ALA	3.2
4	A	174	ILE	3.1
4	A	293	ILE	3.1
4	A	262	LYS	3.1
4	A	247	GLU	3.1
4	A	250	TYR	3.1
4	A	314	ASP	3.0
4	A	298	ILE	3.0
4	A	10	THR	3.0
4	A	206	LYS	2.9
4	A	269	VAL	2.8
4	A	183	ARG	2.8
4	A	306	VAL	2.8
4	A	299	ARG	2.8
4	A	202	SER	2.7
4	A	283	ARG	2.7
4	A	325	TRP	2.7
4	A	200	PHE	2.7
4	A	152	ARG	2.6
4	A	335	GLU	2.6
4	A	7	PRO	2.6
4	A	290	GLY	2.6
4	A	199	SER	2.6
4	A	319	ILE	2.5
4	A	278	PHE	2.5
4	A	334	SER	2.5
4	A	173	TYR	2.5
4	A	238	VAL	2.5
4	A	237	GLY	2.4
4	A	302	GLY	2.4
1	T	13	DC	2.4
4	A	282	MET	2.4
4	A	291	PHE	2.4
4	A	273	THR	2.2
4	A	11	LEU	2.2
4	A	297	THR	2.2
4	A	181	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	320	PHE	2.1
4	A	6	ALA	2.1
4	A	315	SER	2.1
2	P	2	DC	2.1
4	A	323	ILE	2.1
4	A	225	THR	2.1
4	A	242	PRO	2.0
4	A	187	SER	2.0
4	A	304	THR	2.0
4	A	76	PHE	2.0
4	A	235	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	D	342	1/1	0.70	0.17	-0.48	54,54,54,54	0
5	NA	A	341	1/1	0.97	0.12	-2.83	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.